

# Thermodynamics of the planar Hubbard model

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The thermodynamic properties: specific heat, entropy, spin susceptibility  $\chi_s$  and charge susceptibility  $\chi_c$  are studied as a function of temperature and doping within the two-dimensional Hubbard model with various  $U/t = 4 - 12$ . Quantities are calculated using the finite-temperature Lanczos method with additional phase-averaging for a system of  $4 \times 4$  sites. Results show that the entropy at low  $T$  reaches a maximum near half-filling at the electron density  $n \sim 1 \pm 0.15$  in the whole regime of studied  $U/t$ . The pseudogap in  $\chi_s(T)$  becomes clearly pronounced for  $U/t \geq 8$  while  $\chi_c$  shows a maximum close to half-filling. The relation of results to those within the  $t$ - $J$  model and to experiments is discussed.

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The Hubbard model is the simplest prototype Hamiltonian for correlated electrons. It has been and still remains the subject of numerous theoretical investigations in connection with the metal-insulator transition [1], the interplay between the magnetism and the itinerant character of electrons, and possible superconductivity emerging solely from the electronic mechanism. A particular attention has been devoted to the two-dimensional model (2D) on a square lattice, expected to capture the physics of superconducting cuprates. A lot of effort has been put into the numerical studies of the ground state properties, using various quantum Monte Carlo (QMC) methods [2].

On the other hand, there are rather few studies of the 2D Hubbard model at finite  $T > 0$ , in particular away but close to the half filling, i.e. at the electron densities  $n \sim 1$ . In the latter regime the minus-sign problem prevents the application of the QMC method at low  $T$  in large systems [2]. Gross features of the specific heat  $C_V(T)$  have been obtained via the internal energy  $E(T)$  using the QMC [3]. Results reveal the evidence of at least two energy scales at large  $U/t \gg 1$ , the larger one representing the upper Hubbard band. The behavior at low  $T$  shows a marked difference between an insulator at half filling  $n = 1$  with  $C_V(T) \propto T^2$ , and an anomalous metal at finite hole doping  $n_h = 1 - n > 0$  (or analogous electron doping). Within the metallic regime the QMC method was so far not able to reach temperatures below the exchange scale  $J \sim 4t^2/U$ , which sets up an characteristic energy of spin dynamics and is thus essential for establishing the low- $T$  physics at low doping. The uniform spin susceptibility  $\chi_s(T)$  has also been calculated [4] using QMC, with even larger restrictions (smaller systems) at finite doping  $n \neq 1$ , and by Dynamical Cluster Approximation [5]. On the other hand, low- $T$  properties of the Hubbard model with  $U \gg t$  are believed to map well on the properties of the  $t$ - $J$  model which is projected on the basis space without doubly occupied sites. Several static and dynamic properties of the planar  $t$ - $J$  model have been recently calculated and followed well into the regime  $T < J$  using the finite temperature Lanczos method (FTLM) [6, 7]. Two most relevant conclusions on the thermodynamic properties of the 2D  $t$ - $J$  model [8] are: a) normal-state entropy

density  $s(T < J)$  is maximum at the 'optimum' hole doping  $n_h \sim n_h^*$  where  $n_h^* \sim 0.15$  at  $J/t = 0.3$ , b) a pseudogap temperature  $T^*(n_h)$ , experimentally (among alternatives) defined with the maximum in the uniform spin susceptibility  $\chi(T)$  [1, 9, 10], shows up also in the  $t$ - $J$  model where  $T^*(n_h)$  decreases with doping and vanishes at the 'optimum' one, c) even at quite low  $T \ll J$  and in the 'underdoped' regime  $n_h < n_h^*$  some thermodynamic properties are close to the behavior of a semiconductor-like nondegenerate fermion gas [11].

Our aim is to obtain thermodynamic results within the planar Hubbard model, which is numerically (for an exact diagonalization approach) clearly more demanding relative to the  $t$ - $J$  model. We list some relevant questions which we address in the following: a) are there any qualitative differences between the thermodynamic properties of the planar  $t$ - $J$  model and the Hubbard model at large  $U/t$ , b) how does the entropy 'optimum' doping shift with decreasing  $U/t$ , c) is there a pseudogap scale also at smaller  $U/t$ .

We investigate the Hubbard model given by

$$H = -t \sum_{\langle ij \rangle s} (c_{is}^\dagger c_{js} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where  $c_{is}^\dagger$  ( $c_{is}$ ) and  $n_{is}$  are creation (annihilation) and number operators for electrons, respectively, and the sum  $\langle ij \rangle$  runs over pairs of nearest-neighbor sites. We limit our calculations to  $U/t = 4, 8, 12$ , where values range from the modest  $U < W$ , smaller than the bandwidth  $W = 8t$ , to the strong correlation regime  $U > W$ . Note that the latter case corresponds to the physics of cuprates where the spin exchange  $J \sim 4t^2/U \sim 0.3 t$ .

We study numerically the Hubbard model on a square lattice using the FTLM [6, 7], based on the Lanczos procedure of exact diagonalization and a random sampling over initial wavefunctions. The advantage in the case of thermodynamic quantities is that they can be expressed solely in terms of a grand-canonical average of conserved quantities ( $k_B = 1$ ), i.e.,

$$\langle f \rangle = \text{Tr} f(N_e, S_z, H) e^{-(H - \mu N_e)/T} / \text{Tr} e^{-(H - \mu N_e)/T}, \quad (2)$$

where  $N_e$ ,  $S_z$  and  $\mu$  refer to the number of electrons, the total spin and the chemical potential, respectively. In the case of quantities as in Eq.(2), the FTLM does not require the storage of Lanczos eigenfunctions, but only of Lanczos eigenenergies  $\epsilon_j^n$ , where  $j = 0, \dots, M$  ( $M$  represents the number of Lanczos steps) while  $n = 1, \dots, R$  runs over random initial Lanczos wavefunctions. We refer for the details of the method to Refs.[7, 8]. Using FTLM in the above way we are able to investigate the model on the lattice of  $N = 4 \times 4 = 16$  sites with periodic boundary conditions.

The main limitation to the validity of results comes from finite-size effects. The latter can be substantially reduced by employing the boundary condition (flux) averaging [12]. In a system with periodic boundary conditions the latter is achieved by introducing the uniform vector potential  $\vec{\theta}$  modifying the hopping elements  $t \rightarrow \tilde{t}_{ij} = t \exp(i\vec{\theta} \cdot \vec{r}_{ij})$ . We use furtheron  $N_t$  uniformly spaced phases  $\vec{\theta}$  instead of a fixed  $\theta = 0$ . In this way results are essentially improved at lower  $U < W$ . This is particularly evident for noninteracting electrons with  $U = 0$ , where results on small lattices otherwise reveal pronounced finite-size effects. In this case, using  $N_t \gg 1$  most properties discussed here become exact even on a finite-size lattice.

Still the main restriction in the thermodynamic validity of our results comes from finite-size effects which show up at  $T < T_{fs}$  where they start to dominate results [7]. In the particular parameter space  $U/t = 4 - 12$ , the 'optimum' cases are at  $n \sim 1 \pm n_h^*$  with  $n_h^* \sim 0.15$  (coinciding with largest entropy  $s = s_{max}$ ) where  $T_{fs}/t \sim 0.1 - 0.15$ . On the other hand,  $T_{fs}$  increases towards  $n = 1$  and  $n \rightarrow 0, 2$ , respectively [7]. Since the properties of the Hubbard model (1) on a bipartite lattice are symmetric around half-filling we present results only for the hole-doped regime  $n_h = 1 - n \geq 0$ .

Using Eq.(2) we directly evaluate within FTLM the electron density  $n = \langle N_e \rangle / N$ , the entropy density  $s$ , expressed as

$$s = \ln \Omega / N + (\langle H \rangle - \mu \langle N_e \rangle) / NT, \quad (3)$$

and the spin susceptibility  $\chi_s = \langle (S_z)^2 \rangle / NT$ . Quantities calculated as functions of  $\mu$  and  $T$  can be consequently presented as well as in terms of  $n$  and  $T$ . Using above quantities we also evaluate the specific heat  $C_V = T(\partial s / \partial T)_\mu$  and the charge susceptibility - electron compressibility  $\chi_c = (\partial n / \partial \mu)_T$ .

Let us first discuss FTLM results for an overall behavior of the specific heat  $C_V(T)$  (per unit cell), as shown in Fig. 1 for  $U/t = 0 - 12$  in the whole relevant  $T$  regime. At high  $T > 0.5 t$  our FTLM results in general agree with those obtained previously with the QMC method [3]. The advantage of FTLM is that we can reach lower  $T \sim T_{fs} \sim 0.1 t$ , well below the exchange scale  $T \ll J \sim 4t^2/U$ . The main message of Fig. 1 is that  $C_V$  reveals the existence of (at least) two energy scales which are well separated for  $U \gg t$ , i.e. for  $U = 12 t$ . The upper maximum is related to excitations within the upper Hubbard band and is well pronounced near half-filling. For a larger doping, i.e. for  $n < 0.85$ , these excitations merge with the lower Hubbard band. At lower  $U = 4 t$ ,

the upper maximum is only weakly present even at  $n = 1$ , and disappears at smallest available doping  $n_h = 0.95$ . Note also that at  $U = 4 t$ , apart from  $n = 1$ ,  $C_V$  merges even quantitatively with the noninteracting result,  $U = 0$  (properties at  $U = 0$  in Figs. 1 - 4 are calculated for an infinite lattice). When discussing the relation of presented results to those within the  $t$ - $J$  model we point out that the upper scale (upper Hubbard band) is projected out in the latter so results for  $C_V$  are typically different for  $T > t$ . [8].

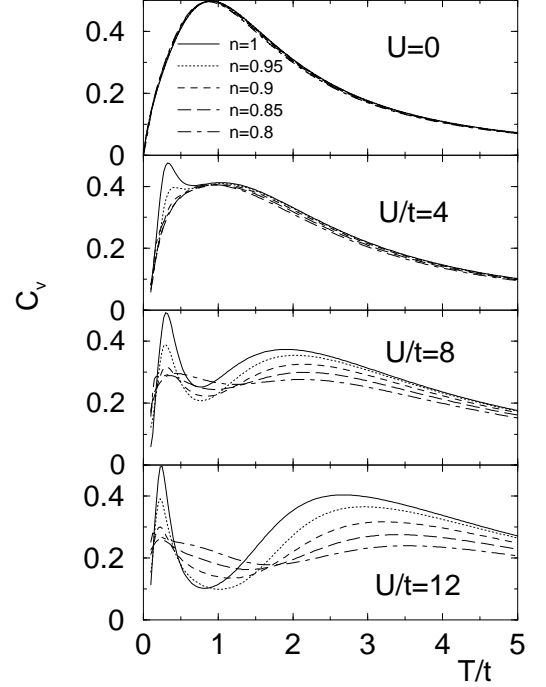


Figure 1: Specific heat  $C_V$  (per unit cell) vs.  $T$  for various electron densities  $n$  near half-filling and different  $U/t$ .  $U = 0$  result is calculated for an infinite lattice.

In the following we focus on the lower energy scale which is essential for the understanding of quasiparticle and low- $T$  properties. In Fig. 2 we show entropy density  $s$  as a function of electron density  $n$  for different  $U/t = 0 - 12$  as well as for few lowest  $T/t = 0.1 - 0.3$ . First observation is that  $U > 0$  leads to an increase of  $s$ , which is largest at an intermediate doping  $n_h = n_h^* \sim 0.15$ . As expected, results for  $U = 12 t$  are even quantitatively close to the ones within the  $t$ - $J$  model [7, 8] with the corresponding  $J = 0.3 t$  where the maximum  $s$  has as well been observed at  $n_h^* \sim 0.15$  and such a doping has been identified as an 'optimum' one. We should note that such a characterization of 'optimality' does not seem to be in conflict with the usual one related to highest  $T_c$  since experimentally in several cuprates the maximum in  $T_c$  and in the entropy [13] appear to be quite close in doping. Plausibly,  $n_h^*$  can be related to the most frustrated case where the kinetic energy of holes (preferring an ferromagnetic ordering) and the spin exchange (favoring antiferromagnetism) are competing and therefore one could expect  $n_h^* \propto J/t$ . Moreover, it is evident from Fig. 2 that the 'optimal' doping  $n_h^* \sim 0.15$  is

quite insensitive to  $U$  in a broad range  $U/t = 4 - 12$ .

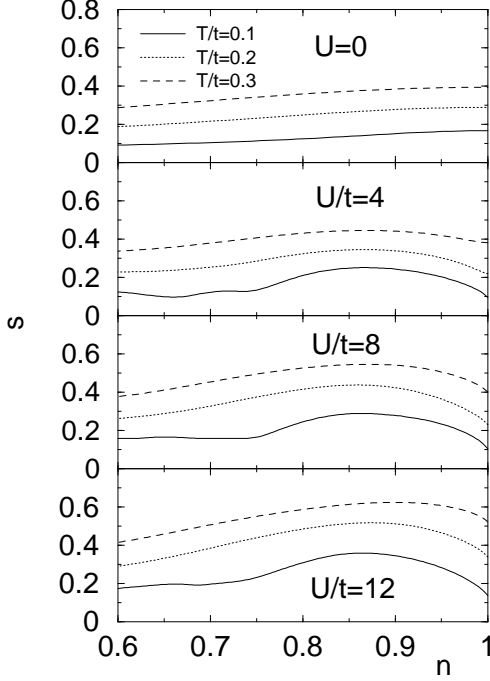


Figure 2: Entropy density  $s$  vs. electron density  $n$  for low  $T/t = 0.1 - 0.3$  and different  $U/t$ .

In Fig. 3 we present results for the spin susceptibility  $\chi_s(T)$  for various dopings close to half-filling  $n = 0.8 - 1.0$  and  $U/t = 0 - 12$ . We first note that here the phase averaging method brings substantial improvement. This is evident by comparing Fig. 3 with QMC results on the same  $4 \times 4$  lattice [4] obtained at a fixed phase  $\theta = 0$ .

As expected, the onset of  $U > 0$  leads to an increase of  $\chi_s(T)$  at lower  $T < t$ . It is however more interesting to follow the development of pseudogap features with increasing  $U/t$ . One of experimental definitions of the (large) pseudogap temperature is related to the maximum  $\chi_s(T = T^*)$  [9]. In fact,  $T^*$  defined in this way matches well with other experimentally established crossovers [1, 10]. It has been found [7, 8] that  $T^*(n_h)$  determined in this way within the  $t$ - $J$  model matches well experiments. As foreseen from the mapping to the  $t$ - $J$  model with  $J = 0.3t$ , we find in Fig. 3 essentially the same behavior for the Hubbard model with  $U/t = 12$ . On the other hand, the pseudogap maximum becomes shallower for  $U/t = 8$ , although the location  $T^*(n)$  does not seem to shift substantially. The pseudogap features disappear at  $U/t = 4$ .

Let us finally comment on results for the charge susceptibility  $\chi_c = dn/d\mu$ , as presented in Fig. 4. For noninteracting electrons at  $U = 0$ ,  $\chi_c$  is essentially  $T$ -independent (except very close to  $n = 1$ , due to the van-Hove singularity) and is equal to the single - electron density of states at the Fermi energy  $\chi_c = \mathcal{N}_F$ . Well away from half-filling, i.e. in the 'overdoped' regime'  $n < 0.8$ , the effect of  $U > 0$  is only quantitative to reduce  $\chi_c$ . This can be attributed to an overall decrease of the effective density  $\mathcal{N}(\epsilon)$  due to the transfer of

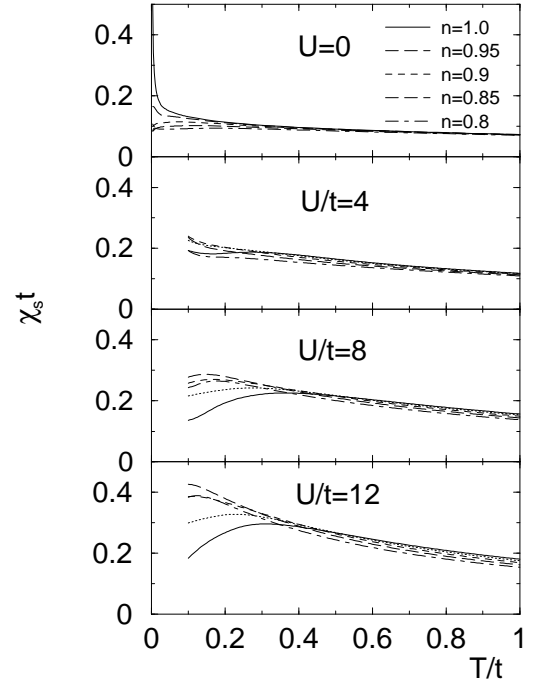


Figure 3: Spin susceptibility  $\chi_s t$  vs.  $T$  for  $n = 0.8 - 1.0$  and different  $U/t$ .

states into the upper Hubbard band. We also note in Fig. 4 that at the same time  $U > 0$  leads to an even flatter variation of  $\chi_c(n)$ .

More indicative and challenging is the development within the 'underdoped' regime  $n_h < n_h^*$ , with a pronounced  $T$  and doping dependence. Very close to half-filling  $n \sim 1$ , we are at  $T > T_{fs}$  dealing with chemical potential  $\mu$  within the charge (Mott-Hubbard) gap. A small density of charge carriers  $n_h \ll 1$  in this regime behaves as in a doped nondegenerate semiconductor, (as established within the  $t$ - $J$  model at low doping [11]) where

$$n_h \sim P e^{-(\mu - \epsilon_v)/T}. \quad (4)$$

Consequently, we get  $\chi_c = n_h/T$ . Such a behavior is evident in Fig. 4, quite universally for all  $U > 0$  and its validity extends at lowest  $T$  up to  $n_h \sim 0.1$ . A large increase in the maximum  $\chi_s$  at low  $T$ , being again rather insensitive to  $U/t$ , is a clear manifestation of strong correlations and of the increasing effective density of states  $\mathcal{N}_F^c$  on approaching the metal-insulator transition. In fact, it has been claimed on the basis of the  $T = 0$  QMC results [1] that within the Hubbard model the charge susceptibility diverges approaching the half-filling as  $\chi_c \propto (1 - n)^{-1/2}$ . The latter is qualitatively consistent with the flattening of the chemical potential as a function of doping  $\mu(n \rightarrow 1)$  in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  observed via the ARPES measurements [14]. Nevertheless, at given lowest  $T \sim T_{fs} \sim 0.1t$  we cannot distinguish a scenario with an enhanced but finite  $\mathcal{N}_F^c$  at  $T = 0$  from a divergent behavior.

Let us summarize some essential conclusions of the present study of thermodynamic properties of the planar Hubbard

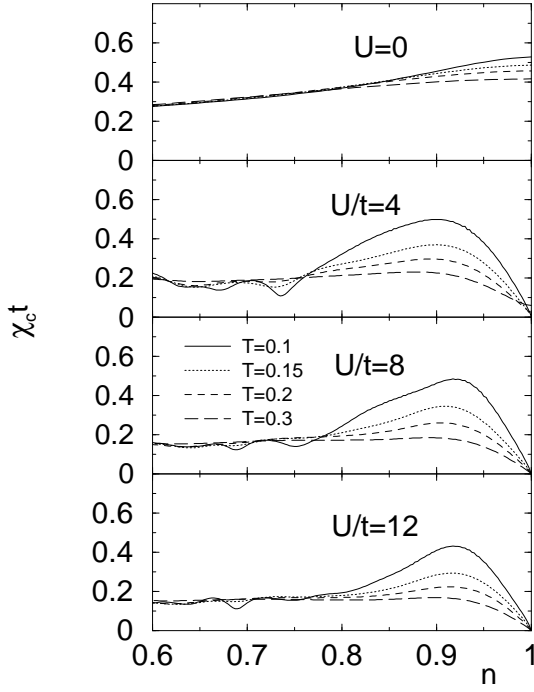


Figure 4: Charge susceptibility  $\chi_c t$  vs.  $n$  for  $T/t = 0.1 - 0.3$  and different  $U/t$ .

model:

- a) The FTLM seems to have advantages with respect to QMC and other numerical methods for the calculation of thermodynamic quantities away from half filling. The phase averaging method used in this study represents an essential improvement and to large extent reduces finite-size effects, in particular at moderate  $U < W$ . Using the FTLM and a phase averaging we reach in our study the low- $T$  regime, i.e.  $T < \tilde{J}$ , where  $\tilde{J}$  is an effective scale where the spin exchange is fully active.
- b) At large  $U/t \gtrsim 12$  results for the thermodynamic quantities match even quantitatively those of the corresponding  $t$ - $J$  model (with  $J \sim 4t^2/U$ ) [7, 8] in the low temperature  $T < t$  window. Excitations into the upper Hubbard band contribute significantly only at large  $T > t$ . On the other hand, for smaller  $U \lesssim 8t$  both scales start to merge, and become inseparable for  $n \neq 1$ . In this intermediate  $U$  regime there is still a qualitative but not a quantitative resemblance to low- $T$  results within the  $t$ - $J$  model. Finally, results for  $U \lesssim 4t$  approach the behavior of noninteracting fermions.
- c) The effective exchange scale  $\tilde{J}$  seems to determine the 'optimal' doping for the entropy maximum  $s(n = 1 - n_h^*) = \max$  as well as the pseudogap scale  $T^*(n_h)$  in  $\chi_s(T^*) = \max$ . It is clear that only at large  $U$  we observe  $\tilde{J} \sim J \sim 4t^2/U$ . On the other hand, for  $U < 12t$  we see that the positions of extrema in  $s(n)$  and in  $\chi_s(T)$  are quite insensitive to  $U/t$ , indicating a rather constant  $\tilde{J} \lesssim 0.3t$  as well as the 'optimum' doping  $n_h^* \sim 0.15$ . The former fact can be understood in terms of less localized character of spin degrees, which leads to an effective spin exchange interaction reduced relative to the large  $U$  expression  $J = 4t^2/U$ .

d) The pseudogap feature (maximum) in  $\chi_s(T)$  is well visible at  $U = 12t$ , but remains only weakly pronounced at  $U/t = 8$  and finally vanishes for smaller  $U$ . This is consistent with the interpretation that the (large) pseudogap  $T^*$  is related to an onset of short-range antiferromagnetic correlations, which are only weakly pronounced for  $U \lesssim 8t$  away from half-filling  $n < 1$ .

e) One expects also an analogous pseudogap in the specific-heat coefficient  $\gamma(T) = C_V(T)/T$  [13], where a depletion should appear at  $T < \tilde{T}^*(n)$ . It is evident that such an effect is present within the model, since near half-filling we see  $C_v \propto T^2$  while at larger doping  $n_h \rightarrow n_h^*$  we get  $C_v \propto T^\nu$  with  $\nu \leq 1$ .

f) We should note that the maximum in  $\chi_s(T)$  is not specific for the 2D Hubbard model, but seems to be generally present also in the 1D model [15]. Nevertheless, in a 1D system there is no qualitative change in the character of low-energy (spin and charge) excitations on doping since the excitations have all the way a linear dispersion and consequently a nonvanishing  $\gamma(T \rightarrow 0)$ , in contrast to a 2D system.

g) Previous studies of thermodynamic quantities within the  $t$ - $J$  model [7] have shown that results (at  $J/t = 0.3$ ) are even quantitatively in agreement with the experimental ones in hole-doped cuprates, in particular the doping dependence of the entropy  $s$  [13], the spin susceptibility  $\chi_s$  [9] and chemical potential  $\mu$  [14]. Our results show essentially equivalence of the low- $T$  behavior of the  $t$ - $J$  model and Hubbard model with large  $U \gg t$ , hence the correspondence with experiments applies again. However, we have shown that many results do not change significantly in a broader range of  $U$ , i.e. there is even a quantitative similarity of  $s(t)$ ,  $n_h^*$ ,  $T^*(n_h)$  etc., so the agreement with experiments persists also in a broader range of  $U/t$ .

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